

2-Methylhexane
591-76-4 | DTXSID5052256

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.32e-05 mol/L

Global applicability domain: Inside

Local applicability domain index: 9.64e-01

Confidence level: 8.58e-01

Nearest Neighbors from the Training Set

Image not found

2-Methylhexane

Measured: 2.53e-05

Predicted: 4.32e-05

Image not found

3-Methylhexane

Measured: 4.94e-05

Predicted: 4.20e-05

Image not found

2,4-Dimethylpentane

Measured: 5.49e-05

Predicted: 4.61e-05

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Pentane,3,3-dimethyl-

Measured: 5.91e-05

Predicted: 4.77e-05